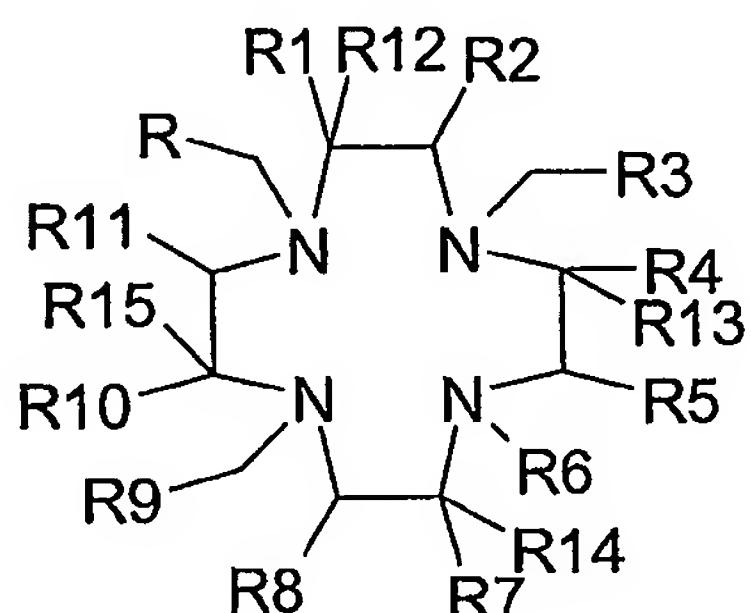


We claim:

1. A compound comprising a polyazamacrocyclic compound and at least one phosphonic group substituted on at least one of the aza groups of said polyazamacrocyclic compound.
- 5 2. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (II):



(II)

where  $R^1 = R^2 = R^7 = R^8 = R^{10} = R^{11} = H$ ;

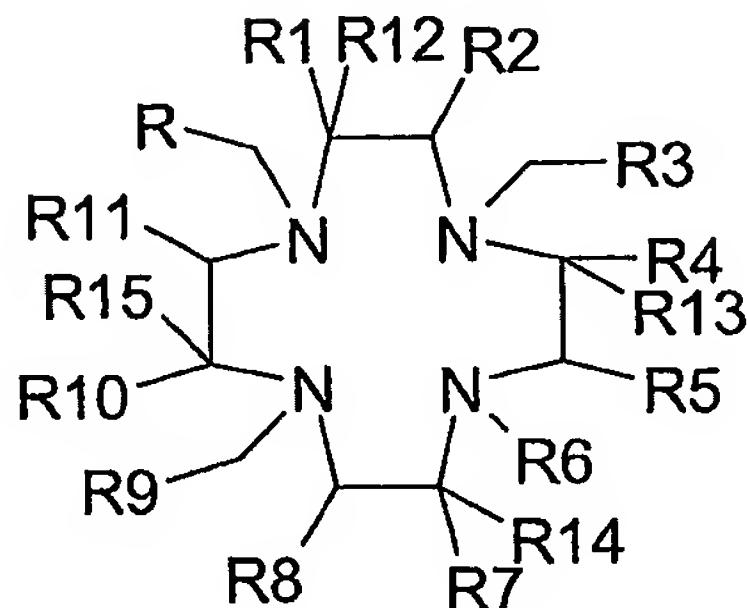
10  $R^{12}, R^{13}, R^{14}$ , and  $R^{15} = CH_3$  or  $H$ ;

$R^4 = R^5$ ; and  $R^{10} = R^{11}$  can be  $H$  or groups taken together forming a cyclic  $C_3$ - $C_4$  alkene group;

15 at least one of  $R, R^3, R^6$  or  $R^9 = X$ , where  $X = CH_2P(O)(OH)_2, CH_2P(O)(OC_4H_9-t)_2, CH_3CHP(O)(OH)_2, CHP(O)(OH)_2-$   
 $(CH_2)_nCO_2H, CHP(O)(OH)_2, (CH_2)_nNH_2, CHP(O)(OH)_2-$   
 $Aryl-CO_2H, CHP(O)(OH)_2-Aryl-NH_2$  or  $CHP(O)(OH)_2-$   
 $Aryl-NHCS$ , where  $n = 1-12$ ; and

when  $R, R^3, R^6$  or  $R^9$  are not  $X$ , then that  $R, R^3, R^6$  or  $R^9$  is  $CO_2C(CH_3)_3$ , or  $CO_2H$ .

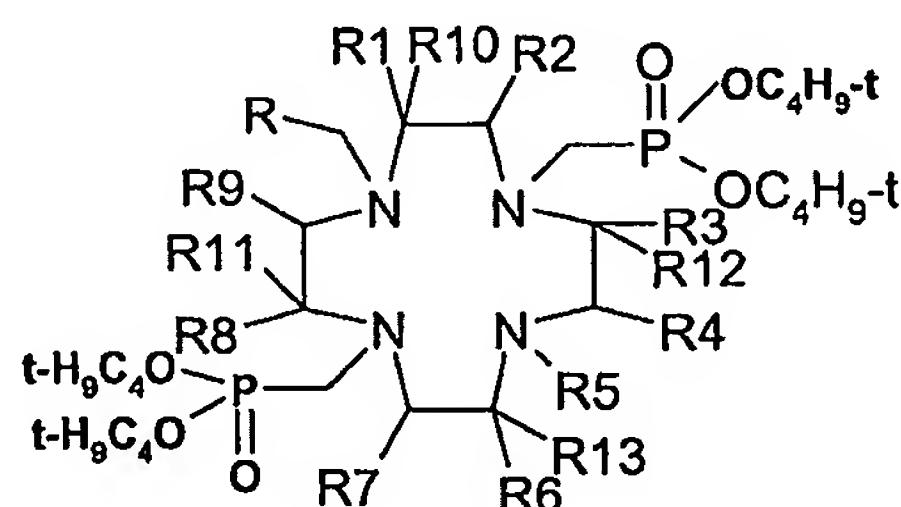
3. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (III):



(III)

5 where  $R = R^3 = R^9 = CO_2 C (CH)_3$ , or  $CO_2 H$ ;  
 $R^1 = R^2 = R^4 = R^5 = R^7 = R^8 = R^{10} = R^{11} = H$ ;  
 $R^{12}, R^{13}, R^{14}$ , and  $R^{15} = CH_3$  or  $H$ ;  
 $R^{10} = R^{11}$  can be  $H$  or groups taken together forming a cyclic  $C_3-C_4$  alkene group; and  
10  $R^6 = CH_2P (O) (OH)_2, CH_2P (O) (OC_4H_9-t)_2, CH_3CH P (O) (OH)_2, CH$   
 $P (O) (OH)_2-(CH_2)_nCO_2H, CH P (O) (OH)_2, (CH_2)_nNH_2, CH P$   
 $(O) (OH)_2$ -Aryl- $CO_2H$  or  $CH P (O) (OH)_2$ -Aryl- $NH_2$ , where  $n$   
= 1-12.

4. The compound of claim 1 wherein said polyazamacrocyclic compound  
15 comprises the general formula (IV):



(IV)

where  $R^1 = R^2 = R^3 = R^4 = R^6 = R^7 = R^8 = R^9 = H$ ;

$R^3 = R^4$  and  $R^8 = R^9$  can be H or groups taken together forming a cyclic C<sub>3</sub>-C<sub>4</sub> alkene group;  
 $R^{10}, R^{11}, R^{12}$  and  $R^{13} = CH_3$  or H;  
 $R = CO_2C(CH_3)_3$ ; and  
5  $R^5 = CH_2P(O)(OH)_2, CH_2P(O)(OC_4H_9-t)_2, CH_3CHP(O)(OH)_2,$   
 $CHP(O)(OH)_2-(CH_2)_nCO_2H, CHP(O)(OH)_2, (CH_2)_nNH_2,$   
 $CHP(O)(OH)_2-Aryl-CO_2H, CHP(O)(OH)_2-Aryl-NH_2$  or  $CHP(O)(OH)_2-Aryl-NHCS$ , where n = 1-12.

5. A compound of the formula:

10-Phosphonomethyl-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid (MPDO3A);  
10-(1-phosphonoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid;  
10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid 1,7-bis(1,1-dimethylethyl)ester;  
10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]- $\alpha'$ -(carboxymethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid  $\alpha, \alpha', \alpha''$ -tris(1,1-dimethylethyl)ester;  
20 10-[[1-[Bis(1,1-dimethylethoxy)phosphinyl]-3-carboxy]propyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic  $\alpha, \alpha', \alpha''$ -tris(1,1-dimethylethyl)ester; or  
4,10-Bis[[bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-tetraazacyclododecane-1,7-diacetic (1,1-dimethylethyl)ester.

25 6. A compound comprising a homo dimer, hetero dimer, homo multimer or hetero multimer of the compound of any of claims 1-5.

7. A complex comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal.

8. A method for preparing a complex comprising the step of conjugating the compound of any of claims 1-5 with a paramagnetic or radionuclide metal.

5 9. A method of imaging comprising the steps of:

administering to a patient a diagnostic imaging agent comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal, and imaging said patient.

10. A method for preparing a diagnostic imaging agent comprising the step of adding to an injectable medium a substance comprising the compound of any of claims 1-5.

11. A kit for preparing a diagnostic imaging agent comprising the compound of any of claims 1-5.

12. A kit for preparing a radiotherapeutic agent comprising the compound of any of claims 1-5.

15 13. A method of treating a patient comprising the step of administering to a patient a radiotherapeutic agent comprising the compound of any of claims 1-5 complexed with a therapeutic radionuclide.

14. A method of preparing a radiotherapeutic agent comprising the step of adding to an injectable therapeutic medium a substance comprising at least one compound of any of claims 1-5.

20

15. The compound of any of claims 1-5 further comprising a linking group.

16. The complex of claim 7 further comprising a linking group.

17. The compound of any of claims 1-5 further comprising a targeting moiety.

18. The complex of claim 7 further comprising a targeting moiety.

19. The compound of any of claims 1-5 further comprising a linking group and a targeting moiety.

20. The complex of claim 7 further comprising a linking group and a targeting moiety.

5 21. A salt form of the compound of any of claims 1-5.

22. A salt form of the complex of claim 7.

23. A method for preparing a polyazamacrocyclic compound bound to a linker, targeting moiety, diagnostic moiety or therapeutic moiety comprising the step of:

conjugating a polyazamacrocyclic compound to a linker, targeting moiety,

10 diagnostic moiety or therapeutic moiety with a coupling agent, wherein:

said coupling agent is selected from the group consisting of DCC, HOBT and

HATU,

said polyazamacrocyclic compound comprises one carboxyl group and/or at least one amino group, and

15 said linker, targeting moiety, diagnostic moiety or therapeutic moiety comprises at least one amino or acid functional group.